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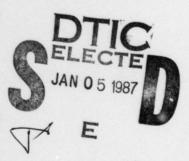
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Task No. NR (243-049)

"Diffusion and Defect Characterization Studies of Mercury Cadmium Telluride"

Principal Investigator: D. A. Stevenson

Department of Materials Science and Engineering Stanford University Stanford, CA 94305



Sponsored by Defense Advanced Research Projects Agency (DOD)

Defense Sciences Office

DARPA Order #5019

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I. Progress During the Report Period

Mercury Cadmium Telluride During the last six month period, progress has continued in the major areas of this program: diffusion studies in Mercury Cadmium Tellurdie (MCT); and growth studies in MCT. The diffusion studies in the present report period have emphasized the experimental determination of interdiffusion at lower temperatures (< 450°C) and the modeling of the defect chemistry of MCT) in order to explain both interdiffusion results and the electrical behavior of MCT. In addition, there is continuing progress on the tracer diffusion studies in MCT. In the crystal growth portion of the program, most of the effort has been devoted to the analysis of our previous work. This has resulted in our submitting four papers to Journals for review, and copies of these manuscripts are enclosed for your information. Work continues on the experimental study of isothermal liquid phase epitaxy (ISOLPE) and on electrochemical studies, A. Diffusion Studies:

In this report period, we have completed the interdiffusion studies of HgTe-CdTe couples from 600°C to 300°C for both Hg-rich and Te-rich conditions. We have analyzed the interdiffusion coefficients (D) as a function of temperature (T) and composition (X) and we proposed that interdiffusion occurs by a dual mechanism in the high temperature region (T \geq 450°C): a vacancy mechanism is dominant in the lower X value region and an interstitial mechanism is dominant at higher X value region. For temperatures below 450°C, we observed a different behaviour from the high temperature region; there is a dependence of D on the component pressures and D increases for higher X values (X \geq 0.5). We attribute this to the predominance of the interstitial mechanism in these lower temperature regions. Our model is confirmed by electrical property studies in the literature (1,2,3,4) and by theoretical calculations of defect concentrations (5).

Progress continues on the topic of tracer diffusion in MCT. We are studying the ${\rm Hg}^{203}$ and ${\rm Cd}^{109}$ tracer diffusion from 500^{0} to 300^{0} C. We find two to three branches in the ${\rm Hg}^{203}$ diffusion profile which are associated with species with different diffusion rates. Since evidence for the fastest species does not appear in the preannealed sample, we chose to reveal the slower branches only. We are investigating the Hg vapor pressure dependence of the two slower branches to establish the diffusion mechanisms for them. Our current results (T \geq 350 0 C) show that the slowest branch is insensitive to Hg vapor pressure, whereas the second fastest depends on Hg vapor pressure in such a manner consistent with a change from a vacancy mechanism to an interstitial mechanism for Ha^{203} when the Hq vapor pressure changes from a Te-rich condition to a Hq-rich condition. Two to three branches were found in the Cd¹⁰⁹ diffusion profile. We also tried to resolve the slower two diffusion processes. The slowest two were independent of the Hg vapor pressure. We are currently analyzing the theoretical relationship between interdiffusion and self-diffusion coefficients for this pseudo-binary sustem, with the objective of explaining the branches that are independent of Hg vapor pressure.

We have finished the Kirkendall effect studies and marker experiment, and hope to interrelate all the diffusion studies.

References

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B. Growth Studies

The isothermal liquid phase epitaxial technique (ISOLPE) was used to investigate the Hg corner of the phase diagram and determine Hg-rich interdiffusion coefficients at 450 and 500° C. Good agreement was obtained in each case with data found in the literature.

A slight modification has been made to the theory for the determination of interdiffusion coefficients from isothermal growth kinetics. The raw data were reanalyzed in the light of this revision and used to fit the interdiffusion coefficient under Te-rich conditions to an equation of the form:

$$D_x(cm^2/sec.) = 300 exp(-7.53X)exp(-1.92eV/kT).$$

Progress continues on the application of the coulometric titration technique to determine free energies of formation of the tellurides at 298°K. Progress has been slow because of the time needed for equilibration. There are also some questions that persist regarding the stability of one of the Li/Te compounds needed for the calculation, because of conflicting information in the literature

II. Planned Activity for the Coming Period.

The work planned for the future emphasizes the following topics: continuation of the experimental tracer diffusion studies; continuation of the analysis of all diffusion results, including a unified theoretical treatment; evaluation of epitaxial growth methods; and continuation of the electrochemical studies of the thermodynamic properties of the MCT system.

III. There were no changes in the key personnel in the report period.

IV. D. A. Stevenson presented a seminar at the Rockwell Science Center on March 10, 1986: "Diffusion and Growth Studies in Mercury Cadmium Telluride,"

M.F.S. Tang and J.G. Fleming presented Research reviews at Ford Aerospace on July 14, 1986.

Two papers were presented at the Ninth Conference on Crystal Growth
June 3-6, 1986, Fallen Leaf Lake, California: Epitaxial Growth of Mercury
"Isothermal Liquid Phase Cadmium Telluride," J.G. Fleming and D.A.
Stevenson

"Interdiffusion and the Kirkendall Effect in the HgTe-CdTe System," M.F.S. Tang and D.A. Stevenson.